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Hydrogen bonds involving C-H groups of 1,1,2,2-tetrabromoethane and their effect on the conformation equilibrium

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Abstract

The solvent and polymer matrix effects on the conformation equilibrium in 1,1,2,2-tetrabromoethane (TBE) are investigated by IR spectroscopy. The free energy differences (ΔG 0) of TBE conformations correlate with the dielectric permittivity function of the medium. A pronounced solvent effect on the absolute integrated intensities of the IR bands arising from the C-H stretching vibrations indicates H-bonding between the C-H groups of TBE and the solvent. The enthalpies of specific interactions due to hydrogen bonding were estimated using the intensity rule (1-3 kcal/mole). The absence of correlations between ΔG 0 and the solvent basicity parameter leads us to conclude that the trans- and gosh-conformers of TBE form nearly equally strong hydrogen bonds. ©1998 Plenum Publishing Corporation.